

Magneto-Stark polaron states in semiconductor quantum wells

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We study theoretically the effect of a lateral electric field on the magneto-polaron states in a quantum cascade laser under a quantizing magnetic field. We show that this problem fits the original Fano model of a discrete state coupled to a continuum, present a detailed analysis of magneto-Stark polaron resonances, and finally discuss the strong consequences on the optical characteristics of an operating structure.

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Nanostructures made of semiconductors are model objects for the study of fundamental interactions in solid-state physics. This results from both the large quantization of their electronic levels and their peculiar response to external fields. Moreover, progresses in growth techniques brought about the concept of spectral engineering, where by a proper multilayer design one is able to construct a desired sequence of levels. Quantum cascade lasers (QCL), which perfectly illustrate this concept, have attracted intense research since their discovery: in there, one realizes a sequence of states allowing population inversion in a region made of a few layers of wells and barriers (the active region) [1]. More recently, it has been shown that a strong magnetic field applied parallel to the growth axis of a QCL structure modifies its emission characteristics [2]. This effect has been associated to the existence of field-induced resonances between Landau levels (LL) of different subbands involved in the population inversion. Inelastic resonances have also been studied, where the magnetic field is chosen so that the two LL's are not resonant but detuned by the energy of one longitudinal optical (LO) phonon [3]. For such field values, one predicts the formation of resonant magneto-polarons (MP) states [4, 5], which are entangled eigenstates issue from the strong coupling between electrons and LO phonons (by the Frölich interaction, prevalent in binary materials often used to fabricate QCL's, like GaAs and InAs). In this work we account for an additional electric field applied perpendicularly to the magnetic field. This is the well-known fields configuration for Hall (classical or quantum) effect [6]. However, we are not interested here in the low-lying states, but shall discuss the effect of the external bias on the highly excited MP states involving the upper lasing level. As we show, this is a model problem, with interest both on the fundamental and applicative sides. Indeed, we demonstrate that it fits the Fano model of a discrete state coupled to a continuum [7]. We demonstrate that the interaction between electrons and LO phonons can be made to evolve continuously from a strong to a weak coupling regime by increasing the electrostatic field. We finally discuss the consequence of this striking qualitative and quantitative bias-triggered evolution of the energy eigenstates on the

optical absorption of a QCL.

Our aim is to describe the magneto-Stark polaron (MSP) states that follow from the interplay of the crossed fields and electron-phonon coupling, and their influence on the QCL optical transitions. For a qualitative rather than a quantitative understanding of the concomitant effects of these three couplings on the QCL functioning, we model its active region by a single quantum well with infinitely height barriers. To start with, let us briefly recall the cases of magneto-Stark states in crossed F and B (in absence of electron-phonon coupling). We consider a quantizing magnetic field applied along the growth Oz direction, described in the Landau gauge $\vec{A} = Bx\hat{y}$, and an electric field applied along the Ox direction. This problem is exactly solvable, with eigenstates [8]:

$$\begin{aligned} \langle \vec{r} | E_l, n, k_y \rangle &= \frac{1}{\sqrt{L_y}} e^{ik_y y} \chi_l(z) \varphi_n(x + \lambda^2 k_y - \frac{v_D}{\omega_c}), \\ \varepsilon_{l,n,k_y} &= E_l + \left(n + \frac{1}{2}\right) \hbar \omega_c - eF \lambda^2 k_y - \frac{1}{2} m^* v_D^2 \end{aligned}$$

where m^* is the electron effective mass, $\lambda = \sqrt{\hbar/eB}$ the magnetic length, $v_D = F/B$ the drift velocity, $\omega_c = eB/m^*$ the cyclotron frequency, χ_l the l -th QW subband wavefunction, k_y the wavevector along the Oy direction (of macroscopic size L_y) and φ_n the n -th Hermite function. We consider a QW width $L_z = 12.33\text{nm}$, which gives a laser emission around 8.7 nm between the first two subbands of a GaInAs-based structure ($m^* = 0.05m_0$ and $E_2 - E_1 = 147.5\text{meV}$). As it is well known, the electric field lifts the LL degeneracy related to the plane-wave motion along Oy , generating an ensemble of crossed magneto-Stark levels, and induces a drift motion of the electron perpendicular to both fields.

In this work we are interested in the effect of the electrostatic field on the magneto-polaron (MP) states. Indeed, it has been shown in previous works, done at $F = 0$ [4, 5], that electrons in a QW subjected to a high magnetic field strongly couple to Longitudinal Optical (LO) phonons by the Frölich interaction [9] $V_{e-ph} = \sum_{\vec{q}} \left(V_q e^{-i\vec{q}\cdot\vec{r}} b_{\vec{q}}^+ + h.c. \right)$, where $b_{\vec{q}}^+$ is the creation operator for LO phonons with wavevector

\vec{q} and $V_q = i\sqrt{e^2\hbar\omega_{LO}(\varepsilon_\infty^{-1} - \varepsilon_s^{-1})/(2V_{cr}\varepsilon_0q^2)}$ with V_{cr} the crystal volume. We assume dispersionless phonons with energy $\hbar\omega_{LO} = 33.7\text{meV}$, and take $\varepsilon_\infty = 11.1$ and $\varepsilon_s = 13.1$ for the high-frequency and static relative dielectric constants, respectively. At $F = 0$, MP states are resonantly formed at the fields $B_p = m^*(E_2 - E_1 - \hbar\omega_{LO})/(pe\hbar) = B_1/p$, where the p -th ($p = 1, 2, \dots$) LL from the E_1 subband with one LO phonon occupancy crosses the $n = 0$ LL of the E_2 one. Following the development of [4, 5], we look for MP states around $B = B_p$ at $F \neq 0$ in the form:

$$|\Psi\rangle = a_d|\varphi_d\rangle + \sum_{q_y} b_{q_y}|\nu_{q_y}\rangle, \quad (1)$$

where

$$|\varphi_d\rangle = |E_2, 0, k_y\rangle \otimes |0_{LO}\rangle, \quad E(|\varphi_d\rangle) \equiv E_d = \varepsilon_{2,0,k_y}$$

$$|\nu_{q_y}\rangle = \frac{\sum_{q_x, q_z} \alpha_{q_x, q_z}(k_y, q_y) |E_1, p, k_y - q_y\rangle \otimes |1_{\vec{q}}\rangle}{\sum_{q_x, q_z} |\alpha_{q_x, q_z}(k_y, q_y)|^2},$$

$$\begin{aligned} \alpha_{q_x, q_z}(k_y, q_y) &= V_q^* \langle E_1, p, k_y - q_y | e^{-\vec{q} \cdot \vec{r}} | E_2, 0, k_y \rangle \\ &= V_q^* \langle \chi_1(z) | e^{-iq_z z} | \chi_2(z) \rangle \\ &\quad \times \langle \varphi_p(x - \lambda^2 q_y) | e^{-iq_x x} | \varphi_0(x) \rangle \\ &\quad \times e^{iq_x(\lambda^2 k_y - v_D/\omega_c)}, \\ E(|\nu_{q_y}\rangle) &\equiv E_{q_y} = \varepsilon_{1,p,k_y-q_y} + \hbar\omega_{LO} \\ &= E_d - \Delta E + eF\lambda^2 q_y, \end{aligned} \quad (2)$$

whit $\Delta E = E_2 - (E_1 + p\hbar\omega_c + \hbar\omega_{LO})$ is the B -dependent detuning ($\Delta E(B_p) = 0$). We have used explicitly the fact that k_y remains a good quantum number for the magneto-Stark polaron (MSP) states, and dropped it from the labelling of $|\Psi\rangle$ and the coefficients a and b . Thus, for a fixed k_y value, we have a Fano problem of coupling (by the Fröhlich interaction) of a discrete state (of energy E_d) to a field-induced continuum (centered at $E_d - \Delta E$ and of spectral width $W = 2\pi\hbar v_D/a_0$, since q_y varies continuously in the interval $(-\pi/a_0, \pi/a_0)$, with a_0 the crystal unit cell). This problem exactly fits the one treated by U. Fano in its original work [7]. The energies fulfil

$$\begin{aligned} E &= E_d + \Delta_p(E) + z_p(E)\Gamma_p(E), \\ \Delta_p(E) &= \text{P} \int dq_y \frac{K_p(q_y)}{E - E_{q_y}}, \\ \Gamma_p(E) &= \int dq_y K_p(q_y) \delta[E - E_{q_y}], \\ K_p(q_y) &= \frac{L_y}{2\pi} \sum_{q_x, q_z} |\alpha_{q_x, q_z}(k_y, q_y)|^2, \end{aligned} \quad (3)$$

where P is the principal part and the phase-shift term $z_p(E)$ is defined from the first equation. We show in figure 1 the functions $\Delta_p(E)$ (figure 1(a)) and $\Gamma_p(E)$ (figure

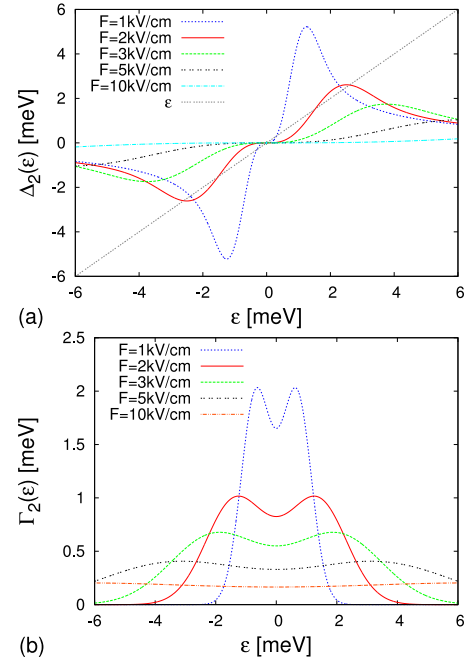


FIG. 1: (Color online) Functions Δ_2 (a) and Γ_2 (b) as functions of the energy $\varepsilon = E - E_d$ for different values of the electric field F , at the $p = 2$ resonance ($B_2 = 24.6T$).

1(b)) for $B_2 = 24.6T$ and different electric fields. This figure shows that, even though the spectral width of the F -induced continuum can be very large as compared to the cyclotron energy ($W \approx 10\hbar\omega_c$ for $F = 2\text{kV/cm}$ and B_2), its effective spectral width, as dictated by the energy range where the matrix elements $K_p(q_y)$ is sizeable, is much narrower for low fields. This justifies using in the construction of $|\Psi\rangle$ only states related to the two quasi-resonant LL's. The energy positions of a Fano resonance fulfills $E - E_d = \Delta_p(E)$. As can be easily seen graphically in figure 1(a), there are actually five solutions at low fields (up to $\approx 2\text{kV/cm}$): one at $E = E_d$ and four resonances symmetrically disposed around E_d . We plot in figure 2 the energies of the MSP resonances as a function of the electric field, for various magnetic fields B_p . One can show that $K_p(q_y)$ is an even function of q_y ; it straightforwardly results that there is an odd number of resonances: $E = E_d$ is always a solution for $F \neq 0$, and there is possibly also an even number of solutions, disposed symmetrically with respect to the energy origin. The solution at the origin is the only possible at high fields, i. e., above a critical field F_p that increases with increasing B_p . Below this critical field, we obtain additionally two (for $p = 1$) or four (for $p \geq 2$) non-trivial MSP resonances, which display a “butterfly”-like shape when plotted as a function of F . In the following we discuss the origin of this butterfly spectrum and show that it follows from two main ingredients: (i) the passage from a strong to a weak electron-phonon coupling regime with increasing electric field, and (ii) the energy-dependence of the matrix elements $K_p(q_y)$.

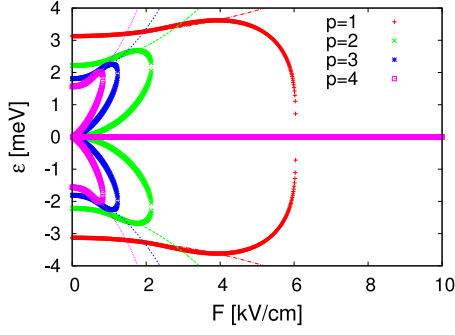


FIG. 2: (Color online) energy position of the Magneto-Stark polaron resonances as functions of the external electric field, for a few magnetic fields B_p ($p = 1-4$; $\varepsilon = E - E_d$). Broken lines: low electric field approximation (see text).

In order to understand the previous results, it is worth recalling that for $F = 0$ the continuum is flat and the electron-phonon interaction is by essence strong. As shown in [4, 5], at resonance field B_p , its diagonalization generates a highly degenerated set of non-interacting one-phonon states at the energy E_d and two split MP levels at energies $E_d \pm \hbar\Omega_p$, where $\hbar\Omega_p$ is the polaron coupling strength. This latter represents the average coupling to the flat continuum and increases with magnetic field: $\Omega_p \propto \sqrt{B_p}$. However, some states of the continuum enter with more weight in the formation of the MP state, as becomes clear by considering the x -related integral in Eq. (2) (let us take $q_x = 0$, for simplicity): the overlap of the two displaced harmonic oscillators wavefunctions is maximum when the displacement is of the order of the extension of their wavefunctions, i.e., $\lambda^2 q_y \approx \sqrt{2p+1}\lambda$. The external bias gives a finite width to the continuum by shifting differently states with different q_y values (by $E_{q_y} - E_d = eF\lambda^2 q_y$). One expects then that the strong coupling regime at the origin of the $F = 0$ magneto-polaron states survives to the applied bias provided that the states with larger coupling strengths are not significantly shifted, i.e., for $eF_p\lambda^2 q_y \leq \hbar\Omega_p$. These two results lead to $eF_p\lambda\sqrt{2p+1} \approx \hbar\Omega_p$, which has a simple physical interpretation: the critical electric field is such that the electrostatic potential drop along the Landau orbit equals the average electron-phonon interaction. We have checked that this simple analysis is in very good agreement with the full numerical calculus of F_p . Finally, at low fields the energy positions of the MP resonances are given by: $\hbar\Omega_p \left[1 + (2p+1)(eF\lambda/(2\hbar\Omega_p))^2\right]$; these quadratic shifts are also plotted in figure 2.

The previous analysis explains the existence of a critical electrical field and the initial quadratic shift of the MP state in figure 2, but does not explain the existence of a vanishing waist in the butterfly profile for $p \geq 2$. The lower branch follows from the particular form of the matrix elements $K_p(q_y)$. Indeed, around B_p , one has ap-

proximately (using $Q = \lambda q_y$):

$$K_p(Q) = \lambda \frac{\hbar^2 \Omega_p^2}{2^{p+1} p! \sqrt{2\pi}} \left(\sum_{n=0}^{p-1} G(p, n) Q^{2n} + Q^{2p} \right) e^{-Q^2/2},$$

$$G(p, n) = \frac{p!(2(p-n-1))!(p-n)(4p-4n-1)}{2^{p-n-1} n! ((p-n)!)^2}.$$

Thus, K_p is a continuously decreasing function of Q for $p = 1$, but presents a camel-back shape for $p \geq 2$ (see the $\Gamma_2(E)$ curves in figure 1(b)). This gives rise to a linear (for $p = 1$) and to a slower (sub-linear for $p \geq 2$) increase of $\Delta_p(E)$ near the energy origin, and thus to the additional butterfly branches that extrapolate to E_d when $F \rightarrow 0$. These additional resonances thus reflect the internal structure of the coupling strength, as opposed to a structureless matrix element often used in problems involving a discrete state coupled to (and placed inside) a continuum.

Let us now consider the high field ($F > F_p$) situation. In this case, the electron-phonon interaction can be treated in the weak coupling formalism. The discrete state acquires a finite lifetime τ_p , given as:

$$\frac{1}{\tau_p(F)} = \frac{2\pi}{\hbar} \Gamma_p(E_d) = \frac{\sqrt{2\pi}}{eF\lambda} \frac{\hbar^2 \Omega_p^2}{2^{p+1} p!} G(p, 0),$$

a result that can of course also be obtained by taking V_{e-ph} as a perturbation in the Fermi's golden rule. It represents the dissociation, triggered by the electron-phonon coupling, of the zero-phonon initial state into the continuum of one-phonon states spanned by the electrostatic field. In conclusion, although not acting directly on the phonon degrees of freedom, the external bias affects the strong electron-phonon coupling at the origin of the MP states in QCL's at high magnetic fields, by rendering the latter resonances at weak fields, and allowing the irreversible emission of one phonon at high fields. This continuous passage from the strong to the weak coupling regimes is thoroughly handled by our non-perturbative model.

In order to demonstrate the influence of these results on the optical properties of a QCL structure, let us consider the absorption of light by electrons in the lowest LL of the ground subband, i.e., in the states $|E_1, 0, k_y\rangle$. For light of frequency ν propagating in the plane layer and polarized along the Oz axis (the usual configuration in operating QCL's), the absorption coefficient towards the high-energy MSP states $|\Psi\rangle$ is proportional to $|a_d[E = E_d + \hbar(\nu - \nu_{QW})]|^2$, where

$$|a_d(E)|^2 = \frac{\Gamma_p(E)}{[E - E_d - \Delta_p(E)]^2 + [\pi\Gamma_p(E)]^2},$$

and $\hbar\nu_{QW} = E_2 - E_1$ (this is because of the selection rules of the dipolar coupling, which preserves both the electron in-plane degrees of freedom and the phonon states [10]). In absence of electron-phonon coupling and the absorption profile is a delta like centered at $\nu = \nu_{QW}$. We

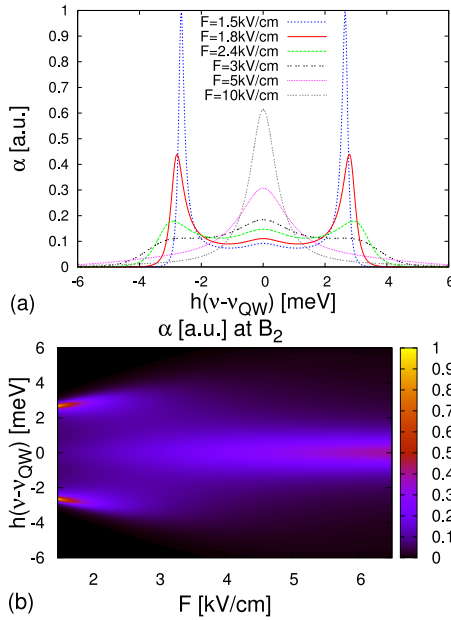


FIG. 3: (Color online) Optical absorption spectra at $B_2 = 24.6T$. (a): energy spectra for different in-plane electric fields. (b): intensity-plot evolution with the applied bias.

show in figure 3 the evolution of the absorption intensity as a function of the light detuning $\nu - \nu_{QW}$ and the electric field, at the B_2 resonance. The electron-phonon interaction and the applied bias enormously affect the absorption profile. We clearly see at very low fields two marked absorption peaks related to the MP states at $F = 0$, which increasingly broaden with increasing F and becomes a faint trace for $F > F_p$, and a single line around the energy origin, which is very broad and weak for $F < F_p$ but gain intensity and sharpens considerably with increasing F .

Let us finally quote some additional remarks. First, the calculations were performed for an InGaAs-based structure, which suffers from an important alloy broadening [5]. However, the same phenomena are expected for GaAs-based samples, with similar material parameters but sensibly free of alloy disorder. Second, it is worth pointing out that the polaron coupling, and thus

the F -induced shift in the absorption spectrum, is in the few meV range for the low p resonances, and thus in principle large enough to be observed in actual samples. Third, the critical field is in kV/cm range, which is high enough to ensure the stability of MP's against unavoidable local micro-field fluctuations in actual samples, and at the same time low enough to prevent important lateral drift during the dwell time of carriers in the active region of an operating QCL. Fourth, we have also calculated the MSP states generated near (but not exactly at) the resonance fields B_p , and obtained that the absorption line shape is affected in a sizeable B -interval around B_p (not shown). Finally, our results suggest that one can sensibly monitor the rate of energy relaxation in the core region of a QCL, by the application of an external modest lateral bias : indeed, MP states are stationary entities that relax only by high-order (anharmonic [11]) processes, comparatively much slower than a direct emission of one LO phonon (few ps versus sub- ps time scales, respectively [11]).

In conclusion, we have considered the magneto-Stark polaron states that result from the interplay of crossed magnetic and electric fields and the electron-phonon coupling in a semiconductor QW. This problem fits exactly the original Fano problem of a discrete state coupled to a continuum, and thus admits an exact solution, in a truncated basis spanned by crossing zero and one-phonon states associated to LL's pertaining to different electron subbands. The model is non-perturbative in either electrostatic and Fröhlich interactions, and describes in an unified way the continuous evolution from a strong to a weak coupling regimes with increasing bias, i.e., the formation of MSP states, which are Fano-like resonances at low fields, and their disintegration at higher fields. Finally, we considered one consequence of such intricate interplay of different couplings on the optical response (absorption spectrum) of a QCL structure and critically considered its possible observation in actual samples.

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